CAFA: A COMPUTER-AIDED CURVE-FIT AND
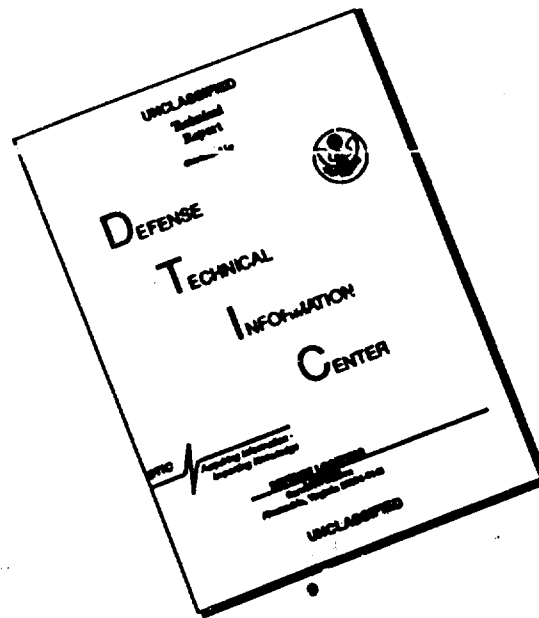
ANALYSIS PROGRAM

AD735946

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ACKNOWLEDGEMENTS

ABSTRACT

The theoretical basis for the CAFA program is discussed. An approximate technique evolving from the theory is applied to the analysis of the current-voltage characteristic of a hypothetical diode, with good results. A printout of the resultant program and data is included.

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INTRODUCTION

The CAFA (Computer-Aided Fit and Analysis; pronounced "café") program was developed for fitting smooth curves to experimental current-voltage and similar data and for using the curves obtained to analyze the data. The original goal was to allow the slope of such curves to be obtained at any point in order to assist in determining the current mechanisms existing in solid-state devices. The program was found to be useful for several other purposes. One, in particular, allowed interpolation between data points. The preliminary results obtained have been encouraging. The program was used extensively to analyze the data discussed in Reference 1.

The subroutine which makes the program possible is the SMOOTH subroutine originally developed by Reinsch (1967), adapted for Fortran by R. E. Jones of Sandia Laboratories, and modified by the author to include interpolation. This subroutine fits a series of spline (cubic) functions to the data points and smooths the transitions between functions by requiring continuity of the first and second derivatives within a certain error chosen by the user. The first and second derivatives are available as printout in addition to the fitted data points and the coefficients of each cubic equation. The latter permitted interpolation between data points. Examination of the program, Fig. 2, reveals the use of these features.

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Several general approaches to determining current mechanisms from the CAFA program are discussed below, along with the specialized version used in this study.

THEORETICAL BACKGROUND

Suppose the current in a diode, I, is given by

$$I = I_o \exp(\beta V/m) \quad , \tag{1}$$

where I_o is constant, $\beta = q/kT$, V is the applied voltage, and m has a constant value.* In this case, the current in the diode is described by one mechanism and the slope of the $\ln(I)$ vs. V curve is

$$\frac{\partial \ln(I)}{\partial V} = \frac{\beta I}{m} \quad . \tag{2}$$

Since everything in Eq. (2) is known except m, m can be determined and the current mechanism can often (but not always) be identified. Unfortunately, total diode currents given by Eq. (1) usually do not exist in practice. The current in real diodes is more often given by an expression of the form

$$I = \sum_i I_{oi} \exp(\beta V/m_i) + \sum_j I_{oj} \exp(V/\phi_j) \quad , \tag{3}$$

where m_i describes the ith temperature-dependent mechanism (e.g., diffusion, space-charge region recombination, surface) and ϕ_j describes the jth nontemperature-dependent mechanism (e.g., tunneling). Even Eq. (3) does not describe the most general current form because it neglects nonlinear effects, such as interactions between current components, plus it

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*To be perfectly general, "current" should be replaced by "flux" and "voltage" should be replaced by "force."

assumes all the I_o's are constant and that $V = V_j$, the junction voltage. Nevertheless, Eq. (?) is often an excellent approximation. For real diodes, one often does not know what the current mechanisms are but could deduce the mechanisms if the m_i's in Eq. (3) were known. If, however, the diode current consists of only two components and is of the form

$$I = I_{01} \exp(\frac{\beta V}{m_1}) + I_{02} \exp(\frac{\beta V}{m_2}) , \qquad (4)$$

then

$$\frac{\partial \ln(I)}{\partial V} = \frac{\beta}{I}(\frac{1}{m_1} + \frac{1}{m_2}) , \qquad (5)$$

and the two values of m cannot be determined easily unless each current type has a clearly defined region of dominance and the experimenter has data covering those regions. Even the simple case of Eq. (5) is not usually seen in practical diodes. To further complicate matters, the value of m describing one mechanism may vary; as an example $2 \leq m < \infty$, depending on injection level, for donor-acceptor pair (DAP) recombination in the space-charge region.[2] A method for finding the value of m at any point, given a current-voltage curve, is therefore desirable. A graphical approach suffers on several counts: It is not accurate enough unless the ln(I) vs. V curve is quite linear, as will be seen below; and it is extremely tedious and time consuming to obtain m at many points. The numerical approach discussed here is quick and gives good results for the special cases discussed.

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Given an experimental current-voltage curve in which the current is presumed to arise from the mechanisms described in Eq. (3), we assume that the current at any point on the curve can be written as

$$I = I_o \exp\left(\frac{\beta V}{m(I)}\right) .$$
(6)

Thus, our basic assumption is that the experimentally-determined current given by Eq. (6) is equivalent to the theoretical current given by Eq. (3). The parameter that allows Eq. (6) to describe the current at any point is, of course, $m(I)$. If $m(I)$ is constant, Eq. (6) reduces to Eq. (1). The slope obtained from Eq. (6) is

$$\frac{\partial I}{\partial V} = \beta I \frac{\partial}{\partial V}\left(\frac{V}{m(I)}\right) .$$
(7)

But $m(I) = m(V)$ implicitly, since $I \propto V$. That is,

$$\frac{\partial}{\partial V}\frac{V}{m(I)} = V\frac{\partial}{\partial V}\frac{1}{m(I)} + \frac{1}{m(I)}\frac{\partial V}{\partial V} ,$$

or

$$\frac{\partial}{\partial V}\frac{V}{m(I)} = V\left[-\frac{1}{m(I)^2}\frac{\partial m(I)}{\partial I}\frac{\partial I}{\partial V}\right] + \frac{1}{m(I)} .$$
(8)

The dependence of m on I will be understood unless otherwise stated.

A differential equation can be obtained that would solve for m in closed form if a closed form solution exists for the

differential equation. By combining Eqs. (8) and (7) we obtain

$$\frac{\partial I}{\partial V} = \frac{\beta I}{m + \frac{\beta IV}{m} \frac{\partial m}{\partial I}} \ . \tag{9}$$

By rearranging Eq. (9) we obtain, since $\partial m/\partial I = dm/dI$ (m is a function only of the current at constant temperature),

$$\frac{dm}{dI} + \frac{1}{\beta IV} m^2 - \frac{1}{V \partial I/\partial V} = 0 \ . \tag{10}$$

This is a very nonlinear d.e. of the form

$$\frac{dy}{dx} + \frac{y^2}{axz} - \frac{y}{bz} = 0 \ , \tag{11}$$

where $x = x(z)$ is known and b ($= \partial I/\partial V$) is known. The d.e. might be solvable using numerical techniques.

We shall briefly discuss the errors which result when the nonlinearity in Eq. (7) is assumed negligible. Considering the derivative on the right-hand side,

$$\frac{\partial}{\partial V} \left(\frac{V}{m}\right) = -\frac{V}{m^2} \frac{\partial m}{\partial V} + \frac{1}{m} \ , \tag{12}$$

which is

$$\frac{\partial}{\partial V} \left(\frac{V}{m}\right) \approx \frac{1}{m} \tag{13}$$

if $\partial m/\partial V$ is negligible. This requires

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$$\frac{1}{m} >> - \frac{V}{m^2} \frac{\partial m}{\partial V} \quad ,$$

so that

$$m >> - V \frac{\partial m}{\partial V} \quad . \tag{14}$$

For $m \approx 2$, $V \approx 1$ volt,

$$\left| \frac{\partial m}{\partial V} \right| << 2 \text{ units/volt.} \tag{15}$$

The rate of change of m with V must be very small for this condition not to be violated. Hence, the approximation that $\partial m / \partial V$ is negligible is often not valid. This approximation is numerically identical to that obtained using an incremental approach which approximates the curve between a series of closely adjacent data points by a set of straight lines, and is approximately equivalent to the results which would be obtained using a graphical technique. Therefore, unless a ln(I) vs. V curve is very linear, a graphical or incremental approach, or an approach which neglects $\partial m / \partial V$ will not suffice for determining the value of m from an experimental curve.

As a special case of the relationship between Eqs. (3) and (6) we write the relation as

$$I = I_0 \exp(\frac{\beta V}{m}) = I_{01} \exp(\frac{\beta V}{m_1}) + I_{02} \exp(\frac{\beta V}{m_2}) . \tag{16}$$

The two terms on the right-hand side of Eq. (16) may be considered as two distinct components or as one distinct component

plus a sum of other components, so that the relation is not necessarily restricted to only two distinct components. This will be called the "two-process" model. We shall assume Eq. (16) holds and determine the effective m vs. V for various ratios R,

$$R \equiv I_{01}/I_{02} \; . \tag{17}$$

R will be constant or nearly so for many situations. Using Eq. (17) we can rewrite Eq. (16) as

$$I = I_{02} \left[R \exp\left(\frac{\beta V}{m_1}\right) + \exp\left(\frac{\beta V}{m_2}\right) \right] \; . \tag{18}$$

The derivative is

$$\frac{\partial I}{\partial V} = I_{02} \left[\frac{R\beta}{m_1} \exp\left(\frac{\beta V}{m_1}\right) + \frac{\beta}{m_2} \exp\left(\frac{\beta V}{m_2}\right) \right] \; . \tag{19}$$

Define

$$f \equiv \frac{I}{\partial I/\partial V} \; ; \tag{20}$$

combining Eqs. (18) and (19) gives

$$f = \frac{R \exp\left(\frac{\beta V}{m_1}\right) + \exp\left(\frac{\beta V}{m_2}\right)}{\beta \left[\frac{R}{m_1} \exp\left(\frac{\beta V}{m_1}\right) + \frac{1}{m_2} \exp\left(\frac{\beta V}{m_2}\right) \right]} \; . \tag{21}$$

Equation (21) can be solved for R:

$$R = -\frac{\frac{\beta f}{m_2} - 1}{\frac{\beta f}{m_1} - 1} \exp\left[\beta V\left(\frac{1}{m_2} - \frac{1}{m_1}\right)\right] . \tag{22}$$

Since R is constant with V, we must have

$$\frac{\partial R}{\partial V} = 0 . \tag{23}$$

Performing the indicated operations on Eq. (22), realizing that $\exp\left[\beta V\left(\frac{1}{m_2} - \frac{1}{m_1}\right)\right] \neq 0$, and rearranging gives

$$\frac{\partial f}{\partial V} = \left(\frac{\beta f}{m_2} - 1\right)\left(\frac{\beta f}{m_1} - 1\right) . \tag{24}$$

This is the criterion for R to be constant. One way to use Eq. (24) would be to find f(V) (from the results of curve-fitting to the I-V characteristic using the SMOOTH subroutine, since this gives $\partial I/\partial V$ also), curve fit to the points f, find $\partial f/\partial V$ from the curve fit and plot the right-hand side and $\partial f/\partial V$ vs. βf on the same curve, using m_1 and m_2 as parameters; one could inspect the results to find integer values of m_1 and m_2 such that the curves intersect. Another way would be to find a second expression describing $\partial f/\partial V$. By differentiating Eq. (20) directly, we obtain

$$\frac{\partial f}{\partial V} = 1 - \frac{I}{(\partial I/\partial V)^2}\frac{\partial^2 I}{\partial V^2} . \tag{25}$$

Since the second derivatives can also be obtained from the curve fit of I vs. V, we have enough information to find $\partial f/\partial V$;

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that is, if the second derivatives are reasonably well behaved. A third method is to rearrange Eq. (24), if $\partial f/\partial V$ can be found, to obtain

$$\beta f = \frac{m_1 + m_2}{2} \quad \frac{1}{2} \sqrt{(m_1 + m_2)^2 - 4m_1 m_2 (1 - \frac{\partial f}{\partial V})} \;. \quad (26)$$

Both sides of Eq. (26) can be plotted vs. V with m_1 and m_2 as parameters. The solutions would be obtained at the curve intersections. For the special case when $\partial f/\partial V = 0$, Eq. (26) reduces to

$$\beta f = m_1 \text{ or } m_2 \;. \quad (27)$$

Thus, one of the m's can be found if $\partial f/\partial V = 0$ somewhere. If $\partial f/\partial V = 1$,

$$\beta f = m_1 + m_2 \text{ or } 0 \;. \quad (28)$$

If $\partial f/\partial V = 1$ and $\beta f \neq 0$, then

$$m_2 = \beta f - m_1$$

if m_1 was found at a point where $\partial f/\partial V = 0$. Still another approach uses f in the differential equation (10). Using the definition of f, Eq. (10) becomes

$$V \frac{dm}{dV} = m - \frac{m^2}{\beta f} \;. \quad (29)$$

If βf is a determinable function, this can be solved to get a family of curves for various V's. Even if f is not a

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determinable function, the expression (26) could be substituted into the d.e. and then one would have a d.e. in terms of m, m_1, and m_2, so that m could be predicted given m_1 and m_2 (a trial-and-error approach). For the special case when $\partial f / \partial V = 1$, the d.e. becomes

$$\frac{dm}{dV} = \frac{1}{V} \left(m - \frac{m^2}{m_1 + m_2} \right) \quad , \tag{30}$$

where we have used Eq. (28) with $\beta f \not= 0$. This can be solved, yielding

$$\frac{m^2 - m_o^2}{2} - \frac{m^3 - m_o^3}{3(m_1 + m_2)} = \ln\left(\frac{V}{V_o}\right) \quad , \tag{31}$$

where m_o is a known value of m at $V = V_o$. This transcendental equation may also be solved graphically.

A somewhat simpler and less tedious approximate approach to determining m_1 and m_2 has been developed and will be discussed next. The approach is useful in a transition region or any region where superposition of two or more current components results in some curvature of the experimental $\ln(I)$ vs. V curve.

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AN APPROXIMATE APPROACH

If the two-process model, Eq. (16), is valid, and if the ln(I) vs. V curve is nonlinear, one may obtain a pair of equations (24) for each two adjacent data points. If the curve is nearly linear, the pair of equations thus obtained may not be linearly independent or may not have a solution, so that the procedure described here will not work in such a region. If a linearly independent pair of equations is obtained, each pair has a unique solution from which the m's can be determined approximately. Since each such pair has a unique solution whether or not the two- or one-process model is valid, values of m can be determined, but these may not be the integer values expected. We define

$$G \equiv 1 - \frac{\partial f}{\partial V} , \qquad (32)$$

$$RPM \equiv \frac{1}{m_1 m_2} , \qquad (33)$$

(the reciprocal product of m's), and

$$SRM = \frac{m_1 + m_2}{m_1 m_2} \qquad (34)$$

(the sum of reciprocals of m's). These symbols are useful computer words. Let I and I + 1 be adjacent data points and look for the Jth solution of the pair of equations obtained from Eq. (24). To be compatible with computer language, let $\beta f \rightarrow$ BF

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and $(\beta f)^2 \rightarrow BF2$. Also rewrite Eq. (24) as

$$G = 1 - \frac{\partial f}{\partial V} = \left(\frac{m_1 + m_2}{m_1 m_2}\right) \beta f - \frac{1}{m_1 m_2} (\beta f)^2 \qquad (35)$$

Then

$$BF(I)SRM(J) - BF2(I)RPM(J) = G(I) \qquad (36)$$

and

$$BF(I+1)SRM(J) - BF2(I+1)RPM(J) = G(I+1) \qquad (37)$$

to a good approximation. The solution of this pair of equations is

$$SRM(J) = \frac{BF2(I+1)G(I) - BF2(I)G(I+1)}{BF(I)BF2(I+1) - BF(I+1)BF2(I)} \qquad (38)$$

and

$$RPM(J) = \frac{BF(I+1)G(I) - BF(I)G(I+1)}{BF(I)BF2(I+1) - BF(I+1)BF2(I)} \cdot \qquad (39)$$

Letting $XM2 \equiv m_2$ and $XM1 \equiv m_1$,

$$XM2(J) = \frac{SRM(J)}{2RPM(J)} - \frac{1}{2RPM(J)} \sqrt{[SRM(J)]^2 - 4RPM(J)} \qquad (40)$$

and

$$XM1(J) = \frac{SRM(J)}{RPM(J)} - XM2(J) \cdot \qquad (41)$$

Once the m's have been obtained, there are nine possible combi nations (which will not be enumerated) of results, wherein m_1

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and m_2 are constants of correct value (i.e., integers), constants of incorrect value, or variables. If one of the m's = 1, the current component may be injection current. If so, its correct I_O can be found as described below. If the other m is, say, 2, where the 2 is found to describe space-charge region recombination current, the I_O found for it may vary, because I_O for such current is, in general, injection-level dependent. This will complicate the results somewhat, but judicious inspection may help in deciphering the results. For any case where one of the m's is not constant, the value of I_O obtained may be treated as a "subtotal" current of the form

$$I_{oi} = I_{oi}' \, \exp(\frac{\beta V}{m}) \, , \qquad (42)$$

where $m = m(I)$. It is possible to treat this subtotal current in the same fashion as the total current: Curve fit to it, assume two current mechanisms and break it up into m_1' and m_2', as before, continuing until the currents have been resolved satisfactorily. The foregoing also applies to any case where one of the m's is constant but incorrect.

In any case, when values of m_1 and m_2 have been obtained, we write

$$I = I_{01} \, \exp(\frac{\beta V}{m_1}) + I_{02} \, \exp(\frac{\beta V}{m_2}) \, . \qquad (43)$$

For two adjacent interpolated data points J and J+1, we have

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$$I(J) = I_{01}(J) \exp\left(\frac{\beta V(J)}{m_1}\right) + I_{02}(J) \exp\left(\frac{\beta V(J)}{m_2}\right) \qquad (44)$$

and

$$I(J+1) = I_{01}(J) \exp\left(\frac{\beta V(J+1)}{m_1}\right) + I_{02}(J) \exp\left(\frac{\beta V(J+1)}{m_2}\right) \qquad (45)$$

to a good approximation, because the I_{oi}'s should be nearly constant between two closely adjacent data points. This pair of simultaneous equations can be solved for $I_{01}(J)$ and $I_{02}(J)$. If $I_{01}(J) = I_{01}(J+1)$, the answers are exact (this will be the case for $m_i = 1$, for example) if the m's are exact. If $I_{01}(J) \neq I_{01}(J+1)$, it does not matter, since a better value will be found on the second iteration. The solutions of Eqs. (44) and (45) are

$$I_{01}(J) = \frac{I(J) \exp\left(\frac{\beta \Delta V}{m_2}\right) - I(J+1)}{\exp\left(\frac{\beta V(J)}{m_1}\right) \left[\exp\left(\beta \Delta V\left(\frac{1}{m_2} - \frac{1}{m_1}\right)\right)\right]} \qquad (46)$$

and

$$I_{02}(J) = \frac{I(J+1) - I(J) \exp\left(\frac{\beta \Delta V}{m_1}\right)}{\exp\left(\frac{\beta V(J)}{m_2}\right) \left[\exp\left(\beta \Delta V\left(\frac{1}{m_2} - \frac{1}{m_1}\right)\right)\right]} \qquad (47)$$

where

$$\Delta V \equiv V(J+1) - V(J) \qquad (48)$$

and we have assumed m_1 and m_2 do not change much between J and J + 1.

To demonstrate two of the approaches which have been used successfully[1] and to test their validity, data from a hypothetical diode were analyzed by the program. This diode had m_1 = 1, m_2 = 2, I_{01} = 10^{-8} units and I_{02} = 1 unit. Its I-V characteristic is plotted in Fig. 1. The resultant computer printout is given in Fig. 2.

In the lowermost and uppermost portions of the curve, where m_2 and m_1, respectively, dominate, Eq. (2) is an excellent approximation. Hence, XM or XMPRIM describes the current mechanisms very well and one could deduce the components easily for this diode. PPRIM is equivalent to I_0 and it is seen to give the correct values at either end of the range.

For the transition region near the center of the curve, the value of m as calculated from Eq. (2) does not give the correct value, as expected. In this region (roughly from subscripts I = 50 to I = 70), the approach using Eqs. (36) through (41) finds its application and the values of m_1 and m_2 are determined with good accuracy in this region. Note also that Eq. (27) can be used to find m_1 and m_2 at the two extremes, since βf (called BFP) $\simeq$ 1 at either end of the curve. The experimental results from real diodes usually do not show large regions of linearity in which Eq. (2) is useful, so that the utility of the latter approach in regions of curvature becomes very apparent. This approach does not work well in the linear

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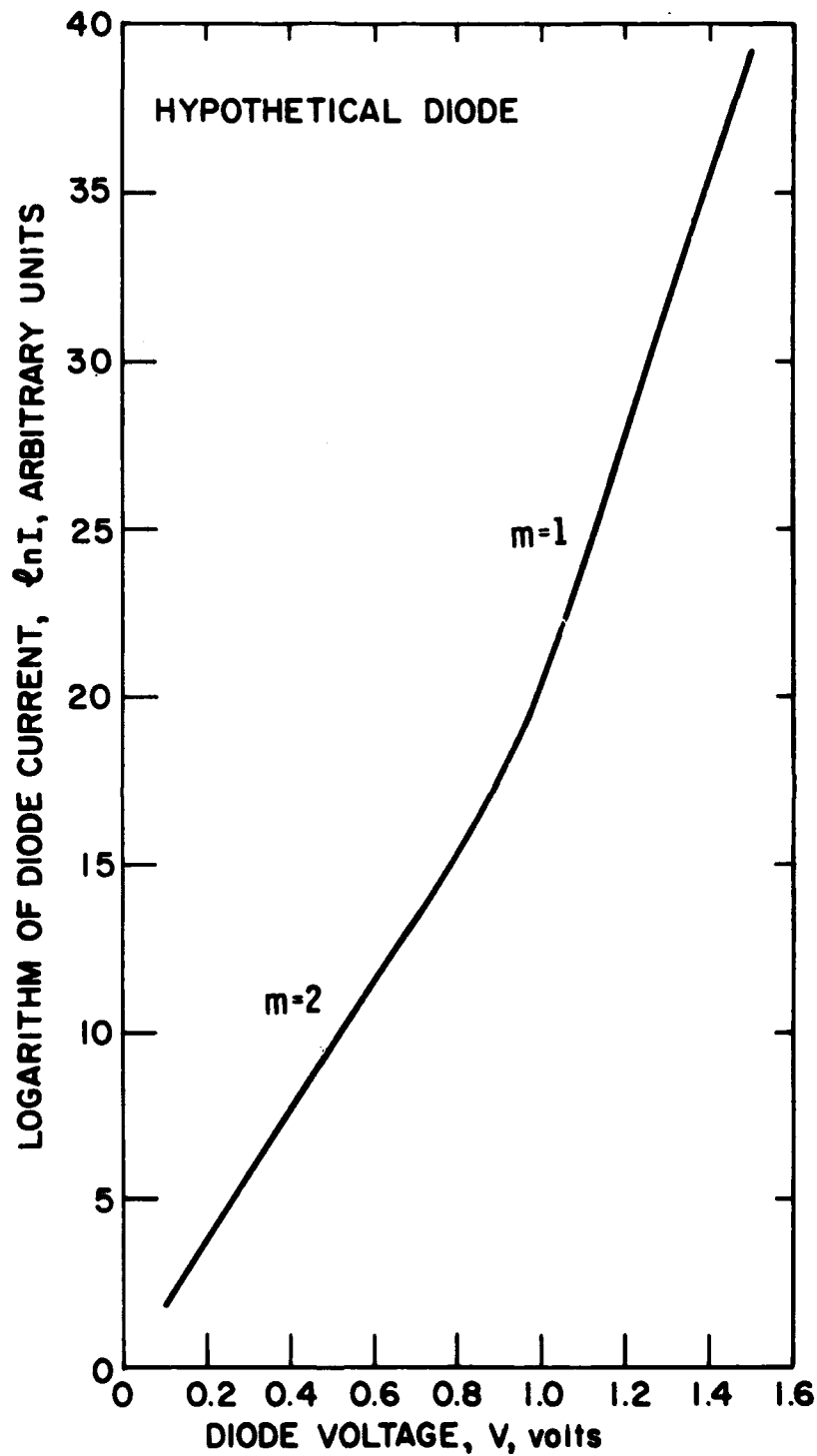
Figure 1.   Current-voltage Characteristic of a Hypothetical
Diode

regions, as discussed earlier. The values obtained in the non-linear region for I_{01} and I_{02} (called CY01 and CY02 or CY01P and CY02P in the program) are not as satisfactory as those obtained for m_1 and m_2. The least error occurs where m_1 (or m_2) passes through its correct value. In this case the error may be negligible (less than 1%), but it may be off by a factor of two or three; however, it is well within an order of magnitude in the worst case, and this would often be adequate. If there is a linear region where m_1 or m_2 is determined correctly, I_{01} and I_{02} will always be calculated within ±20%.

At present, the CAFA program is in a primitive stage of development. Further work should provide a more useful, accurate and flexible program which will be of considerable value in experimental research.


```
C
C
C
C    DESCRIBE DATA FROM CARD FITTED, TO DATA POINTS USING SCATTER S.....
C    ............................................................
C
C    INPUT VOLTAGE DATA, SETTING
C
C    ............................................................
C
C    ARBITRARY INSTRUCTIONS.
C
C    PARAMETER DEFINITIONS.
C
C    DX, Y AND DATA X AND DATA Y(INPUT) VALUES
C    DXI AND DYI ARE ...  OF DX AND DY
C    LY AND CVL ARE CALCULATED Y AND IN CV
C    DRVCV IS DERIVATIVE X,P,T, DX OF CY
C    CVP IS CALCULATED X POINT AS DETERMINED BY INTERPOLATIO...
C    CAPI IS LN OR EXP
C    CVPI IS CALCULATED Y PRIME CORRESPONDING T.. ..P
C    CVPI IS LOG OR CVP
C    DRVCVP IS DERIVATIVE OF CVP
C    META, NDDTM,P,DPDTM,XN AND XNDRTM ARE DEFINED IN SUBROUTINE
C    FITTED.
C
C    THE PARAMETER CARD (3RD FROM BEGINNING) SHOULD BE CHANGED AS REQUIR-
C    ED TO DESCRIBE THE KIND OF DATA BEING FITTED.
C
C    THE 1ST CARD MUST BE CHANGED AS REQUIRED TO READ THE DATA DESIRED.
C    THE CARD 102 SHOULD BE USED ONLY IF A CHANGE IN SCALE IS DESIRED.
C    IF S IS DESIRED IS NOT IN HE END,THE 3RD CARD IN THE MAIN PROGRAM
C    MUST BE CHANGED
C    THE CALL SMOOT- CARD SHOULD READ
C
C        CALL SMOOTH(DX,Y,CV,..DVCV,CVP,CVP,DRVCVP,P, S,FY)
C
C    IF IT,FAW DATA IS USED.
C
C        CALL SMOOT.(CVE,.VI,CV, DRVCVL,CVC,CVVL,DRVCVP,.P, S,FY)
C
C    IF SMOOTING DATA IS USED O.
C
C        CALL SMOOT.(CVE,XVI,CVI,DRVCVI,...P,.P,(DCVPI,DP,P,S,FY)
C
C    IF SMOOTING DATA IS USED.
C    SUMSQUATE FITTED EQUL.. . SMOOTH.
C    ... THE CASE IF SMOOTING A LOG-LOG DATA, CORR... ARE APPLI.. TO THE
C    SMOOTH, A.. BITTED TO CORRECT THE VALUES .....AT BE.... THE CURVE
C    FIT CHECK
C    IT IS READ VALU.S SO THAT THE DERIVED OR THE DATA ...CV OF USED
C    STRAIGHT READ (SEE ON III AND ... 112 GET)..
C
C    THE ...., IN..,...,/ ARE IN AND T... IS NA I UP T. SUIT THE
```

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Figure 2.   The CAFA Program.   Printout for the Hypothetical Diode has been Included.
The PLOTIT Plots have not been Included in order to Save Space.

```
126    XM1(I)=XM1.
127    IF(10.-ABS(XM2P(I)))127,128,128
128    WRITF(6,129)I,XM2P(I)
129    FORMAT(6HO ID = ',I2,' WAS CHANGED FROM ',F11.4,' TO 10.0')
       XM2(I)=10.
120    CONTINUE
       XM1(XP)=10.
       XM2P(I)=10.
       GO 130 I=1,94
       TMLV=XM2P(I)+XM2P(I+1)-REP(I+1)+REP2P(I)
132    IF (TM(-7)131,132,131
135    IF (I-1) 135,135,116
       XM1P(I)=1.
       XM2P(I)=1.
800    WRITF(6,800)
       FORMAT(/,'XM1P(I)AND XM2P(I) +ERE SET+TO 1')
136    6H T4 130
       XM1P(I)=XM1P(I-1)
       XM2P(I)=XM2P(I-1)
801    WRITF(6,801)T
       FORMAT(/,XM1P(I) AND XM2P(I) +EWE SET EQUAL TO THE TH NEXT LOWER
       VALUES FOR I= ',I2)
       GH TO 130
171    SRMP=(REP2P(I+1)+RP(I)-RF2P(I)-RP(I+1))/TMLV
       RPP=(REP(I+1)+RP(I)-RP(I+1)+RP(I+1))/TMLV
       TMLV=SRMP+SRMP+4.+HRMP
       IF(TMLV)132,133,133
133    TMLV=SQRT(TMLV)
       IF (RPMP)134,132,174
134    TMLV=1./(2.+RPMP)
       XM2P(I)=TMLV+(SRMP-TMLV)
       XM1P(I)=-XM2P(I)+SRMP/RP+P
       IF(10.-ABS(XM1P(I)))140,141,141
140    WRITF (6,142)I,XM1P(I)
142    FORMAT(6HO ID = ',I2,' XM1P(I) WAS CHANGED FROM ',F11.4,' TO 10.0')
       XM1P(I)=10.
141    IF (10.-ABS(XM2P(I)))114,144,144
143    WRITF(6,145)I,XM2P(I)
145    FORMAT(6HO ID = ',I2,' XM2P(I) WAS CHANGED FROM ',F11.4,' TO 10.0')
       XM2P(I)=10.
144    CONTINUE
       IF(XM1P(I))8R4,150,130
804    TEMP1=-XM1P(I)
       XM1P(I)=XM2P(I)
       XM2P(I)=TEMP1
835    FORMAT(/,XM1P(I) AND XM2P(I) WERE INTERCHANGED AS I= ',I2,' FOR TH
       IF SIG. OF THE NEW XM2P(I) WAS CHANGED')
130    CONTINUE
       XM1P(150)=10.
       XM2P(150)=10.
       TMLV=XM2P(150)/(-.02*+10.0)
       DO 700 I=1,94
```

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MEMORY MAP

PROCEDURES

LOCAL DYNAMIC

ABSOLUTE

STMNT LABELS

COMMON

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      SUBROUTINE SPL(N,X,Y,DY,H,S,CXP,RPRIM,MIPRI,A,B,IV,H2,H2PRIM)
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C   ABSTRACT
C   SMOOTH FITS A SMOOTH SPLINE THROUGH THE GIVEN SET OF DATA
C   BY MINIMIZING THE INTEGRAL OF THE SECOND DERIVATIVE SUBJECT
C   TO THE CONSTRAINT THAT
C
C   SUM ((W(I)*(Y(I))/DY(I))**2) .LE. S.
C   I=1

```
C
C     DESCRIPTION OF ARGUMENTS
C        N  - NUMBER OF DATA VALUES
C        X  - ABSCISSA ARRAY
C        Y  - ORDINATE ARRAY
C        DY - WEIGHT ARRAY. IF S.EQ.0, DY(I) SHOULD BE AN ESTIMATE
C             OF THE ERROR IN Y(I).
C        S  - SCALE FACTOR FOR WEIGHTS, NORMALLY = N.
C        A,B,C,D - CUBIC BETWEEN X(I) AND X(I+1) IS
C             A(I) + B(I)*H + C(I)*H**2 + D(I)*H**3
C             WHERE H IS DESIRED ABSCISSA MINUS X(I).
C        R  - ARRAY OF SMOOTH SPLINE VALUES
C        R1 - ARRAY OF SMOOTH SPLINE DERIVATIVES
C        H2 - ARRAY OF SMOOTH SPLINE SECOND DERIVATIVES
C        T,T1,U,V - WORK ARRAYS
C
C        X,Y,DY,A,B,C,D MUST BE DIMENSIONED AT LEAST N
C        H,R1,H2,T,T1,U,V MUST BE DIMENSIONED AT LEAST N+2
C
C     REFERENCE -- NUMERISME MATHEMATIK 10,177-151 (1967) C H REINSCH
C        CONVERSION FROM THE ALGOL BY R E JONES, DIV 9422, SANDIA LABS
C        THE ORIGINAL N1 HAS FIXED AT 1 TO AVOID WASTED WORK ARRAY SPACE
C        THE ORIGINAL N2 IS CALLED N HERE
C        ALL WORK ARRAY INDICES ARE 1 LARGER THAN IN THE ALGOL,
C        TO AVOID A ZERO SUBSCRIPT.
C
C        PROGRAM HAS BEEN MODIFIED TO CALCULATE CXP,RPRIM AND MIPRI, WITH-
C        IN THE PROGRAM, INSTEAD OF OUTSIDE....R. HALL,12/1/70
C
      DIMENSION X(25),Y(25),DY(25)
      DIMENSION R(25),R1(25),R2(25),T(25),T1(25),U(25),V(25),A(25),
     1H(25),C(25),D(25)
      DIMENSION CXP(100),RPRIM(100),MIPRIM(100)
      DIMENSION /(100)
      DIMENSION H2PRIM(100)
      COMMON DELTX
C
C     INITIALIZE
      V(1) = 0.0
      R(2) = 0.0
      R1(N+1) = 0.0
      R2(N+1) = 0.0
      R2(N+2) = 0.0
```

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```
      F2= ...
      IF((F2...G5)... GO TO 650
      H = ...
      H = (...-V(2))/(X(2)-X(1)))

      DO ... I=2,M2
      S = ...
      H = (V(I+2)-V(I+1))/(X(I+1)-X(I))
      ...=G-H(I)-R2(I-1)*H(I-1)
      ...
  600 H(I+1) = ...
      H = ...
      IF (H.LT.0.0) GO TO 650
      P = P+(S-F2)/((SQRT(S/F)+P)*H)
      GO TO 250

C     FINISH
  650 DO 700 I=1,N
      A(I)=V(I)-P*V(I+1)
  700 C(I)=C(I+1)

C
      DO 800 I=1,M2
      H=X(I+1)-X(I)
      D(I)=(C(I+1)-C(I))/(3.0*H)
  800 B(I)=(A(I+1)-A(I))/H-(H*C(I)+C(I+1))*H
      H(N)=0.0
      D(N)=0.0

C     OUTPUT DERIVATIVES, ETC.
      DO 900 I=1,M2
      A(I) = A(I)
      B1(I) = B(I)
  900 R2(I) = 2.0*C(I)
      R3(I) = A(H)
      H=X(I)-X(M2)
      A1(I)=(...H(M2)+H2...C(M2)+B(M2))*H+A(M2))
      A2(I)=B(M2)*H+2.0*C(M2)

C     DELTA IS INCREMENT 'DELTA X' ON X AXIS
      DELTA =(X(N)-X(1))/99.
      M=1
      DO 201 I=1,100
      C+X(I)    = X(I))+H*DELTA
      M=M+1
  201 CONTINUE
      T=1
      DO 101 I=1,100
      IF ((X(I)) .GE. X(I+1)) GO TO 101
  101 CONTINUE
```

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MEMORY MAP

PROCEDURES

LOCAL RELATIVE

LOCAL DYNAMIC

ABSOLUTE

STMT LABELS

COMMON

30

NEXT JOB
X

TEMPERATURE 300 DEG.K   NO. OF DATA POINTS IS   0

31

32

34

REFERENCES

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2. L. W. Aukerman and M. F. Millea, Phys. Rev. 148, 759 (1966).